

Claim Amendments

Please cancel, without prejudice or disclaimer, claims 1-9 and 15-21 as drawn to non-elected inventions.

Claims 1-9 (canceled)

Claim 10 (original) A method comprising:

predicting a secondary structure of a protein;

generating a three-dimensional representation of the predicted secondary structure;

optimizing the secondary structure by adjusting dihedral angles using smart moves; and

determining a three-dimensional protein structure by modeling the optimized secondary structure on a topomer model.

Claim 11 (original) The method of claim 10, wherein said secondary structure is a consensus secondary structure prediction.

Claim 12 (original) The method of claim 10, wherein optimization is performed using a random Monte Carlo method.

Claim 13 (original) The method of claim 12, wherein the random Monte Carlo method is used in conjunction with a localized energy function.

Claim 14 (original) The method of claim 10, wherein said three-dimensional structure model is refined using simulated annealing.

Claims 15-21 (canceled)

Claim 22 (new) The method of claim 10, wherein the protein secondary structure is predicted by at least one technique selected from the group consisting of Chou-Fasman, GOR (Garnier,

Osguthorbe and Robson), PSI-pred, JPRED, Prof, PREDATOR, PHD, ZPRED, nnPredict, BMERC, PSA Server, SSP and PROFsec.

Claim 23 (new) The method of claim 10, further comprising determining the permissible ranges of phi and psi dihedral bond angles consistent with the predicted secondary structure for each amino acid residue in the protein.

Claim 24 (new) The method of claim 12, wherein the random Monte Carlo method is performed with or without simulated annealing.

Claim 25 (new) The method of claim 10, wherein optimization is performed using at least one technique selected from the group consisting of Brownian dynamics, random Monte Carlo, molecular dynamics, simulated annealing, molecular mechanics and energy minimization.

Claim 26 (new) The method of claim 10, wherein optimization is performed using at least one program selected from the group consisting of AMBER, X-PLOR, INSIGHTII, CHARMM, DISCOVER and GROMOS.

Claim 27 (new) The method of claim 10, wherein the topomer model is derived using Continuous Configuration Boltzman Biased Direct Monte Carlo Method.

Claim 28 (new) The method of claim 10, further comprising optimizing the topomer model.

Claim 29 (new) The method of claim 28, wherein the topomer model is optimized by simulated annealing to minimize free energy.